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MEASUREMENT OF APPARENT TEMPERATURE IN POST-DETONATION FIREBALLS USING ATOMIC EMISSION SPECTROSCOPY

W. K. Lewis
Sensors Technology Office
University of Dayton Research Institute
Dayton, Ohio 45469

C. G. Rumchik (AFRL/RWME)
Air Force Research Laboratory
Eglin AFB, FL 32542



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Measurement of apparent temperature in post-detonation fireballs using atomic emission spectroscopy

W. K. Lewis^{1,a)} and C. G. Rumchik²

¹*Sensors Technology Office, University of Dayton Research Institute, Dayton, Ohio 45469, USA*

²*U.S. Air Force Research Laboratory, Eglin AFB, Florida 32542, USA*

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The energy release dynamics of explosives are of ongoing interest, but the short timescales involved often limit the measurements that can be made during these processes. We have used atomic emission spectroscopy to measure the temperature of fireballs resulting from detonation of charges of Hexahydro-1,3,5-trinitro-1,3,5-triazine doped with barium nitrate. The time-averaged emission spectra indicate an apparent temperature of ~ 3000 K, in good agreement with theoretical predictions. The technique demonstrated herein should be applicable to time-resolved studies, including those on detonation timescales. © 2009 American Institute of Physics.

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The measurement of energy release and the associated kinetics are of fundamental importance for understanding and controlling exothermic chemical reactions. Although the energy release processes associated with explosives are of ongoing interest, measurements are often made difficult by the fast time scales involved. For gram-scale explosive samples, the detonation wave typically sweeps through the entire sample in several microseconds. The subsequent after-burning of underoxidized detonation products can then produce a fireball that persists for several milliseconds. The fireball often releases more energy than the detonation itself, albeit more slowly.¹ Unfortunately, the time scales associated with these processes limit the measurements that can be made. The high temperatures and pressures involved in explosions also limit measurement options, since any sensors employed must be able to withstand the extreme environment.

To characterize the energy release associated with explosions, it is desirable to determine the temperature and pressure of the system and to date, a variety of techniques have been developed to measure pressure in detonations and fireballs.² On the other hand, temperature measurements have been less extensive, partly because sensors rugged enough to withstand the explosion have response times longer than the phenomena of interest. Atomic and molecular emission spectroscopies would seem to be attractive techniques for temperature measurement, particularly given that they have been used extensively to study the structure and dynamics of flames³ and plasmas.⁴ Additionally, such techniques can be used to measure very fast processes and an emission spectrum can be recorded at a distance from the explosion. The results from several studies utilizing emission spectroscopy in the visible^{5–8} and IR^{9,10} spectral regions to examine explosives have now been reported. We note that while pyrometry methods have also been used to measure temperatures during explosions, recent work suggests that

quantitative interpretation of such data can be problematic without detailed phenomenological knowledge of the emissivity function.¹¹

However, emission spectra obtained from explosions are often complex, with many emission bands, which are frequently overlapping.^{5–10} Additionally, broad emission from incandescent particles can be observed, as well as signals from impurities with strong emission lines. These factors make it difficult to interpret the resulting spectra. An alternative approach is to dope an explosive with an impurity that will produce atomic emissions, which are simpler to interpret, thereby introducing an atomic “thermometer” into the sample. Flames have been studied analogously by seeding thermometric species into burners.^{3,12} Interestingly, Wilkinson *et al.*⁶ have recently observed Al atomic emission lines in the spectrum of aluminum-rich explosives and were able to use these signals to measure the temperature of the vaporized aluminum. However, in these studies the aluminum was present in substantial concentration in order to increase the energy released by the explosive sample. An ideal thermometric impurity would be present only in small concentrations to avoid perturbing the chemical dynamics of the system and minimize the effects of self-absorption. Additionally, candidate thermometric species must produce several strong emission lines in the spectrum that originate from different upper energy levels in order to allow the populations of the associated states to be determined.

Barium nitrate was chosen as a thermometric impurity for the current work since Ba atoms emit several strong well-characterized lines in the visible region that originate from different upper energy levels. Charges of either Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) or RDX doped with a small amount (1 wt %) of barium nitrate were prepared. It is known from slot-burner flame studies that higher concentrations of thermionic impurities become problematic due to self-absorption effects.¹² To prepare the barium-doped explosive charges, barium nitrate was ball milled for several hours to produce a fine powder. The milled barium nitrate was then combined with RDX and a hydroxyl-terminated polybutadi-

^{a)}Author to whom correspondence should be addressed. Electronic mail: lewiswik@notes.udayton.edu.

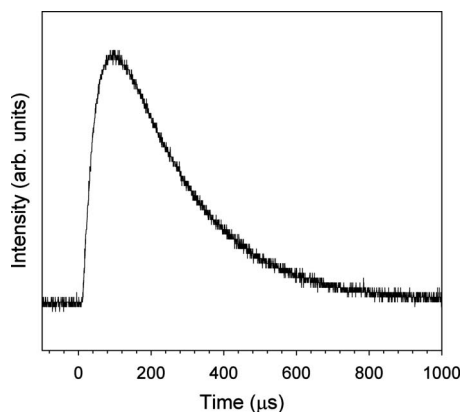


FIG. 1. Typical photodiode trace recording the relative radiance of the fireball generated following detonation of a 40 g charge of RDX.

ene (HTPB) binder and mixed thoroughly. Undoped RDX charges were prepared by mixing RDX with the HTPB binder without barium nitrate. The two mixtures were then pressed into 1 in diameter cylindrical charges of 40 g total mass. Both types of charges contained 6 wt % HTPB binder. The bare charges were then detonated using Reynolds RP-81 detonators.

Light from the explosions was collected using 5 mm diameter collection lenses mounted to the ends of 1000 μm core-diameter fiber optics (Ocean Optics). The collection optics were placed in an observation room located approximately 5 m away from the explosive charges and were aligned to view the center of each charge through a protective BK7 glass view port. The light collected by the fiber optics was sent to a photodiode with a nominal time resolution of 1 ns (Thorlabs Det10A) and a spectrometer with a resolution of ~ 1 nm and a usable spectral range of ~ 460 –800 nm (Ocean Optics USB-4000). We note that in order to avoid saturating the photodiode signal, a neutral density filter was placed between the fiber optic output and the photodiode detector.

The relative radiance of the fireball as a function of time was measured by recording the photodiode signal using a digital oscilloscope (Tektronix). A typical photodiode trace is shown in Fig. 1, where $t=0$ corresponds to the detonator firing signal. Following detonation of the charge, emission from a fireball was observed for several hundred microseconds. Emission spectra during this time were collected by the spectrometer, which was configured to be triggered by the detonator signal. The integration interval of the spectrometer was 5 ms, which captured all of the light output of the fireball. The wavelength and intensity axes of the spectrometer were calibrated before the explosive shots using a mercury-argon lamp (Oriel) and a tungsten-halogen lamp with a known color temperature (Ocean Optics), respectively. Finally, each shot was repeated several times to confirm reproducibility.

In Fig. 2 we show typical spectra collected following detonation of RDX charges [Fig. 2(a)], RDX charges with 1% barium nitrate impurity [Fig. 2(b)], and the difference

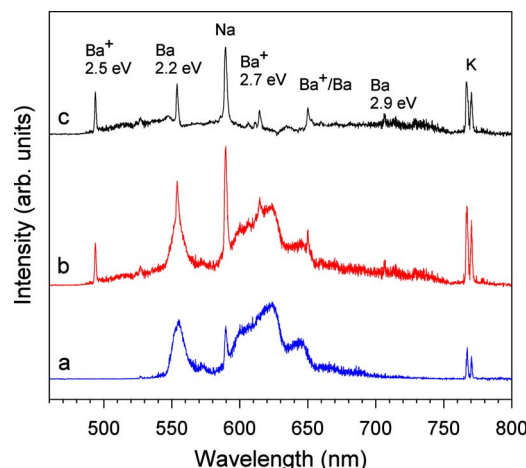


FIG. 2. (Color online) (a) Emission spectra collected following detonation of RDX and (b) RDX doped with 1% barium nitrate by weight. (c) The difference spectrum is also shown and exhibits strong signals from barium atom and barium ion emissions. The apparent temperature of both barium species can be calculated from the relative intensities of the respective emission lines in the difference spectrum.

spectrum [Fig. 2(c)] generated from subtracting the former from the latter. We note that the spectra were subtracted as collected, without employing any scaling procedures. In the spectrum of pure RDX [Fig. 2(a)], we see several broad emissions as well as sharp lines at 589, 766, and 770 nm. The sharp lines most likely result from sodium and potassium impurities.¹³ The broad emissions are more difficult to interpret and likely contain contributions from several vibronic bands, but a full assignment of these emission signals is beyond the scope of this initial investigation. Interestingly, the spectrum appears to be largely free from emissions from incandescent particles, which we would expect to produce a broad gray-body continuum signal. Examination of the spectrum of RDX doped with barium nitrate [Fig. 2(b)] reveals the same complex emission spectrum observed for undoped RDX, except now we also find several well-known emission lines from barium atoms and cations at 493, 554, 614, 650, and 706 nm. We note that the sodium and potassium emissions have also increased in intensity, suggesting that these may be present as impurities in our barium nitrate sample as well.

The difference spectrum [Fig. 2(c)] shows a nearly background-free spectrum in which the atomic emissions from barium atoms and cations are quite clear. We find strong peaks at 554 and 706 nm assigned to the $^1S_0 \leftarrow ^1P_1^0$ and $^3D_3 \leftarrow ^3F_4^0$ transitions in Ba atoms and peaks at 493 and 614 nm assigned to the $^2S_{1/2} \leftarrow ^2P_{1/2}^0$ and $^2D_{5/2} \leftarrow ^2P_{3/2}^0$ transitions in Ba^+ ions, respectively.¹⁴ We note that the peak at 650 nm may have contributions from both $\text{Ba}(^3D_3 \leftarrow ^3D_3^0)$ and $\text{Ba}^+(^2D_{3/2} \leftarrow ^2P_{1/2}^0)$ at the resolution of our spectrometer (~ 1 nm). Since the associated energy levels, degeneracies, and Einstein A coefficients for each of these transitions are well known,¹⁴ we can calculate the apparent temperature from the Boltzmann populations of the energy levels using the two-line method.^{3,6,15} Examining the Ba^+ ion signals at 493 and 614 nm, which originate from states 2.5 and 2.7 eV above the ground state, respectively,¹⁴ we obtain an apparent

temperature of 2800 ± 400 K. Applying the same method to the Ba atom peaks at 554 and 706 nm, corresponding to levels 2.2 and 2.9 eV above the ground state,¹⁴ we find an apparent temperature of 3600 ± 1000 K. The larger uncertainty of this value reflects the lower signal-to-noise ratio of the peak at 706 nm.

Although these values are in agreement within the uncertainty and agree well with the theoretical adiabatic flame temperature of 3150 K (calculated using the method outlined in Ref. 1), we must be cautious in our interpretation of these results since it has been shown that the apparent temperature of a flame may differ by several hundred Kelvin from the average temperature in nonisothermal flames.¹⁶ This is not a serious limitation in the present case, since the spectra shown herein already represent time-averaged results. Additionally, the optical depth of the fireball is not currently known. Nevertheless, these results demonstrate the viability of the basic technique, and future experiments are planned to measure time-resolved temperatures inside detonations and fireballs using spectrometers with improved sensitivity and spectral range. Finally, we believe that this technique may also be useful to measure the temperature of fireballs resulting from complex explosive mixtures, for which calculation of the theoretical fireball temperature is not straightforward.

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